

SUPPLEMENTARY MATERIAL TO  
 **$\pi$ – $\pi$  interactions in structural stability: Role in superoxide  
dismutases**

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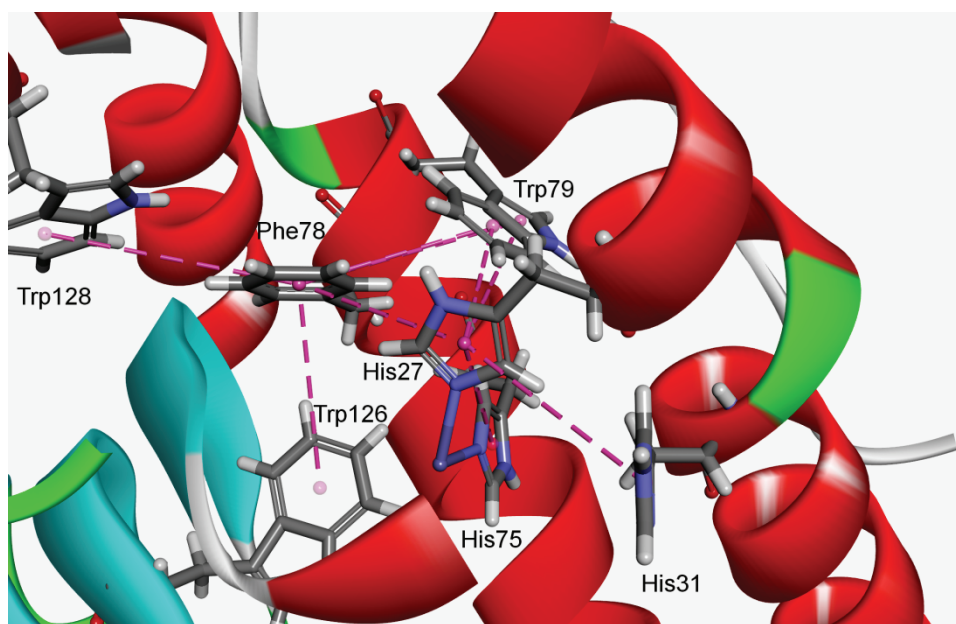


Fig. S-1. Example of a multiple  $\pi$  interactions ( $\pi$ -network) for the cambialistic SOD from *Propionibacterium shermanii* (PDB code 1ar5); The interactions are marked with a pink dashed lines.

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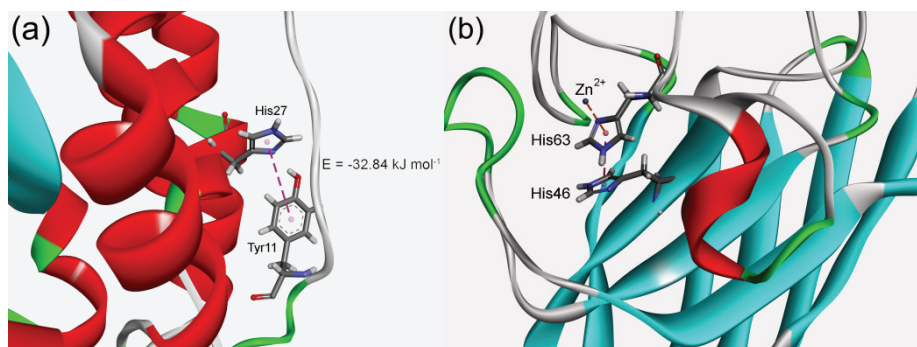


Fig. S-2. Details of  $\pi$ - $\pi$  interactions: a) The strongest attractive  $\pi$ - $\pi$  interaction of *Escherichia coli* MnSOD (PDB code 1d5n). The interaction is marked with a pink dashed line: A:His27-A:Tyr11;  $R_{\text{cen}} = 5.70 \text{ \AA}$ ,  $R_{\text{clo}} = 3.61 \text{ \AA}$ ,  $\theta = 59.77^\circ$ ,  $\lambda = 51.92^\circ$ ,  $E = -32.7 \text{ kJ mol}^{-1}$ ; b) Interaction energy of  $\pi$ - $\pi$  interaction in the presence of metal cation ( $\text{Zn}^{2+}$ ) in Cu/Zn Tomato Chloroplast SOD (PDB code 3pu7): A: $\text{Zn}^{2+}$ -A:His27—A:Tyr11;  $R_{\text{cen}} = 3.97 \text{ \AA}$ ,  $R_{\text{clo}} = 2.98 \text{ \AA}$ ,  $\theta = 26.01^\circ$ ,  $\lambda = 41.21^\circ$ ,  $E = -327.7 \text{ kJ mol}^{-1}$ .